AFOSR-DURIP Final Report: A Computational Cluster for Advanced Plasma Physics Simulations AFOSR Grant # FA9550-08-1-0272

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1 Executive Summary

This DURIP equipment award was used to purchase, install, and bring on-line a computational cluster for plasma physics simulations. An SGI integrated cluster environment "ICE" unit was purchased, featuring 192 2.8 GHz processors (on 24 nodes) with 384 GB high-speed RAM on an Infiniband backbone. Additional nodes include an 8-processor login node (32 GB RAM) and a data server with a 6 TB RAID6 Infiniband system, plus "admin" and "rack leader" nodes. SGI personnel setup the system on-site, with additional integration performed by our local IT personnel. SGI also installed cluster control software and licenses for the SUSE-based Linux operating system.

Software was purchased and installed including Intel Fortran and C/C++ compiler suites (debuggers, performance measurements, etc.), the TotalView parallel debugger, and the MOAB/PBS scheduling software.

Comparisons were made amongst several cluster manufacturers, including Cray, IBM, Dell, Silicon Mechanics, Rackable Sytems, and SiCortex before deciding on the SGI ICE model as the most "turn-key" system. The system was ordered in late 2008 and arrived in early 2009 and was up and running routinely with local users in a few weeks.

Local University of Washington computational groups have made extensive use of the DURIP cluster, running several different advanced extended MHD/two-fluid codes. This DURIP award has greatly increased turnaround time and productivity for these groups.

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Figure 1: Photographs of the SGI ICE cluster. The 24 8-processor compute nodes can be seen in the bottom right (green LEDs). The admin node console monitor is open (video screen) located in front of the login and RAID server nodes.

2 Examples of Usage

The two UW AFOSR computational programs, the "Algorithm Development for the Two-Fluid Plasma" (PI: U. Shumlak, AFOSR Grant # FA9550-05-1-0159) and the AFOSR STTR "Electrodeless Lorentz Force (ELF) Thruster" project (PI: Dr. J. Slough, MSNW L.L.C., Redmond, WA, AFOSR, STTR Phase II FA9550-08-C-0036) subcontract to the University of Washington (PI: B. A. Nelson) have made extensive use of the computational cluster. (These projects are given priority usage.)

Other complementary numerical physics projects, such as the UW Plasma Science and Innovation Center (PSI-Center) have also made use of this cluster.

2.1 Codes Running on the DURIP Cluster

Three main codes have been used on the DURIP cluster for AFOSR projects and by the PSI-Center: WARPX, NIMROD, and HiFi.

2.1.1 The WARPX Code

In the UW-written WARPX code, the multi-fluid plasma equations are formulated in divergence form, which includes source terms. The source terms couple the fluids to the electromagnetic fields, account for collisions between the fluids, and provide sinks and sources from atomic reactions. A high-order algorithm is being developed that solves the complete multi-fluid plasma model such that equilibrium, perturbation, and transient phenomena can be accurately simulated. The algorithm implements the discontinuous Galerkin method to achieve high-order accuracy and will use body-fitted computational meshes to model realistic, general geometries. Novel numerical approaches are being investigated to realize high-order calculations of complex three-dimensional geometries. These numerical approaches include efficient time-integration techniques, such as the Hancock method, and time-integration methods that are not limited by the shortest timescale of the system, such as implicit backward difference and spectral-deferred correction methods. The algorithm will also take advantage of the parallel computing architectures that are available locally, including the new cluster, as well as those at the Major Shared Resource Centers (Dell PowerEdge, Cray XD1, and others). The new algorithm will be benchmarked against known analytical results and experimental data from the Air Force Research Laboratories [the field reversed configuration (FRC) implosions for magnetized target fusion (MTF) at Kirtland AFB and the plasma thruster work at Edwards AFB. The new algorithm will be able to simulate plasma dynamics using more physically accurate models. Simulations performed on the DURIP cluster are shown in Figs. 2 & 3.

2.1.2 The NIMROD Code

The subcontract to the University of Washington (PI: B. A. Nelson) for numerical support of ELF uses the Non Ideal Magnetohydrodynamic with Rotation, Open Discussion code,

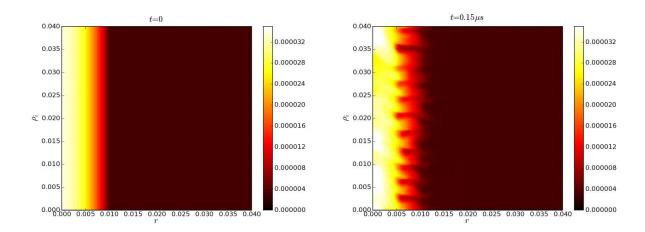


Figure 2: WARPX simulations of a Z-pinch using "realistic" parameters, I=50 kA, $n=1\times 10^{22}$ m⁻³, B=1 T, 1 cm pinch radius in a two-fluid regime, *i.e.* about 3 Larmor radii in the pinch, indicating a small-scale instability when the system is perturbed. Plots are at t=0 and 0.15 μ s.

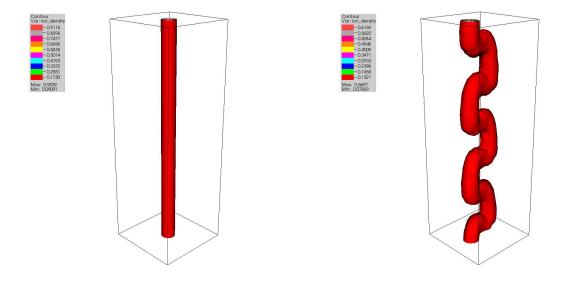


Figure 3: WARPX simulations of astrophysical jets in 3D in an MHD regime, *i.e.* 10 Larmor radii in the narrow pinch, and an asymmetric kink instability develops. Plots are normalized and are at t=0 and 5 Alfvén transit times.

NIMROD[1, 2]. NIMROD is a macroscopic simulation code having several of the critical features for modeling FRC thrusters such as ELF. It has been used for numerical spheromak and RFP studies. NIMROD's algorithm solves compressible nonlinear magneto-fluid equations with electric-field terms selected to represent either the non-ideal single-fluid MHD model or two-fluid models of magnetized plasmas. Solution fields are marched from initial conditions with a semi-implicit algorithm for the MHD equations[3]. The time-centering of velocity is staggered from magnetic field, mass density, and temperature so that the integration of wave-like terms is symplectic. A semi-implicit operator is used to extend the range of numerical stability to arbitrarily large values of $c\Delta t/h$, where c is the magneto-acoustic wave speed, Δt is the time step, and h is the mesh spacing. Temporal truncation errors for wave propagation are then dispersive and not dissipative, which is important for simulating the nearly dissipation-free conditions encountered in astrophysical and laboratory plasmas. In addition, the MHD semi-implicit operator is based on the linear ideal-MHD energy integral[4, 2] for accuracy at large Δt -values.

ELF plasmas are produced using rotating magnetic fields (RMF) in a tapered cylindrical geometry, as simulated on the DURIP cluster using the NIMROD code, Fig. 4.

2.1.3 The HiFi/SEL Codes

The HiFi (high-order finite — spectral — elements) code[5] is a 3D extension of the 2D SEL (spectral elements) code *ibid*. HiFi solves extended MHD equations posed in flux-source form on a finite-element hexahedral grid. Evaluation of mesh generation and efficient parallel solvers have been principally developed on the DURIP cluster.

The AFOSR STTR ELF project has benefited from development and simulations on the DURIP cluster. Neutral fluid was added to the Hall MHD equations in SEL, and demonstrated transfer of momentum from ions to neutrals in a translated FRC, a key design of the ELF thruster. Figure 5 shows an initial FRC equilibrium in a neutral background that is accelerated by external coils. The compression of the FRC ionizes the background neutrals, then expands and accelerates into downstream neutrals. The FRC essentially stops as the ion momentum is transferred to the neutrals which continue moving. This process could be applied continuously to create a directed neutral velocity along with the FRC translation, providing more thrust.

3 Publications and Presentations

The following publications are in preparation that made extensive use of the DURIP cluster:

- E.T. Meier, V.S. Lukin, U. Shumlak, Spectral element spatial discretization error in solving highly anisotropic heat conduction equation, Comp. Phys. Comm., (article in press) 10.1016/j.cpc.2009.12.018
- R.D. Milroy, C.C. Kim, and C.R. Sovinec, "Magnetohydrodynamic Simulations of FRC Formation and Sustainment with RMF Current Drive", in preparation

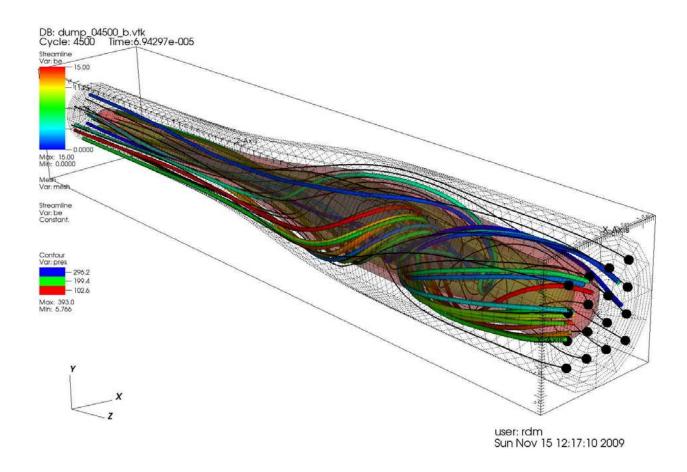


Figure 4: NIMROD ELF simulation results. Magnetic field lines: Colored lines are launched from z=0.3 m and black lines are launched from the end boundary. A partially transparent pressure contour is shown in the background.

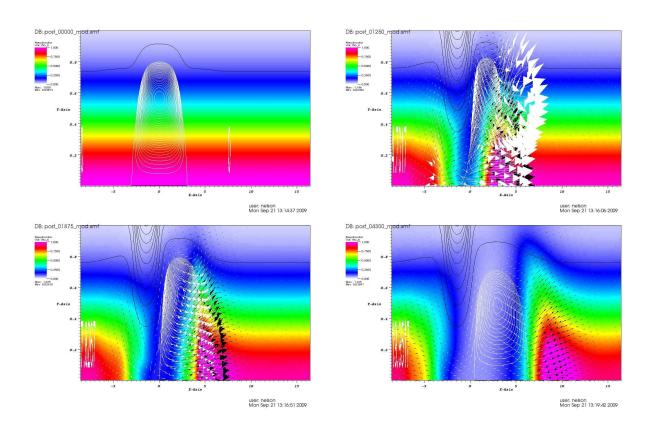


Figure 5: SEL simulations of ion/neutral fluid momentum exchange in for the ELF thruster. White/black line contours are magnetic flux inside/outside the separatrix, pseudo-color contours are neutral density, and momentum density, $\rho \mathbf{v}$, demonstrate transfer from ions (white arrows) to neutrals (black arrows).

- B. Srinivasan and U. Shumlak, "A Semi-Implicit, Ideal, Full Two-Fluid Plasma Model", in preparation
- W. Lowrie, V.S. Lukin, U. Shumlak, "Mesh Deformation Metrics Applied to High-Order Finite (Spectral) Elements", in preparation

My 2009 APS Poster's work and ICC 2010 made use of the ICE cluster:

2009 APS: "Plasma Solution Quality in Distorted, Body-Fitted Meshes in SEL/HiFi", W. Lowrie, V.S. Lukin, U. Shumlak.

2010 ICC: "Multi-block capabilities in HiFi and its application to modeling the ZaP z-pinch experiment". W. Lowrie, V.S. Lukin, U. Shumlak.

The following conference presentations made extensive use of the DURIP cluster:

- R. D. Milroy, C.C. Kim, and C.R. Sovinec, "Nimrod Simulations of FRC Formation with Rotating Magnetic Field Current Drive", poster, APS 2009
- W. Lowrie, V.S. Lukin, and U. Shumlak, "Plasma Solution Quality in Distorted, Body-Fitted Meshes in SEL/HiFi", poster, APS 2009
- E.T. Meier, V.S. Lukin, and U. Shumlak, "Two-fluid plasma-neutral model development and application", poster, Innovative Confinement Concepts Workshop 2010
- R. D. Milroy, C.C. Kim, and C.R. Sovinec, "Nimrod Simulations of FRC Formation and Sustainment with Rotating Magnetic Field Current Drive", invited talk, Innovative Confinement Concepts Workshop 2010
- B. A. Nelson, A.H. Glasser, T.R. Jarboe, C.C. Kim, G.J. Marklin, W. Lowrie, E.T. Meier, R.D. Milroy, U. Shumlak, C.R. Sovinec and J.B. O'Bryan, E. Held, J.-Y. Ji, and V. Lukin, "Simulations of ICC Experiments by the Plasma Science and Innovation Center", invited talk, Innovative Confinement Concepts Workshop 2010
- W. Lowrie, V.S. Lukin, and U. Shumlak, "Multi-block capabilities in HiFi and its application to modeling the ZaP Z-pinch experiment", poster, Innovative Confinement Concepts Workshop 2010

4 Summary

A computational cluster for advanced plasma physics simulations was selected, ordered, installed, and is running routinely. It is gratifying to hear the users of the DURIP cluster comment about the benefits of having a local developmental cluster to provide fast turn around time.

The DURIP proposal included the following as "Synergistic Benefits to DoD":

• Cutting Edge Plasma Physics Simulations

- Accelerated development of two-fluid 3D codes
- Accelerated and more in depth numerical investigation of the ELF project
- Synergy with PSI-Center and NIMROD Team research
- Perform research identified as important by the USAF Scientific Advisory Board[6]
- Education (Graduate and Undergraduate)
 - Both of the sponsored AFOSR grants and the PSI-Center strongly involve graduate and undergraduate students
 - Young scientists will work on cutting edge codes and hardware

These benefits have already been realized.

References

- [1] A.H. Glasser, C.R. Sovinec, R.A. Nebel, T.A. Gianakon, S.J. Plimpton, M.S. Chu, and D.D. Schnack. The nimrod code: a new approach to numerical plasma physics. *Plasma Physics and Controlled Fusion*, 41:747 55, 1999/03/. NIMROD code;toroidal plasma;long-wavelength;low-frequency;fusion plasma;resistive tearing mode;Alfven time;resistive interchange mode;shaped equilibrium;ballooning mode;reversed-field pinch;.
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- [4] K. Lerbinger and J.F. Luciani. A new semi-implicit method for mhd computations. Journal of Computational Physics, 97(2):444 – 59, 1991/12/. compressional fast magne-toacoustic waves;semi-implicit method;MHD computations;nonlinear three-dimensional resistive MHD equations;unconditionally stable;shear Alfven waves;nonlinear physical plasma phenomena;high spatial resolution;longtime simulations;.
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